Abstract Submitted
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First-Principles Approach to Transient Heat Flow in Quantum Systems[1] KAMIL WALCZAK, Department of Chemistry and Physical Sciences, Pace University, One Pace Plaza, New York City, NY 10038, KIRK YERKES, Aerospace Systems Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH 45433, NANOSCALE PHYSICS DIVISION TEAM, THERMAL MANAGEMENT CENTER COLLABORATION — We examine heat transfer via quantum advection modes (coherently correlated quantum states) between two thermal baths of different temperatures mediated by quantum system with discrete spectrum of accessible energy levels. Nanoscale transport is treated within the first-principles method by including the superposed wave functions into the quantum expression for heat flux. Our results show the specific modifications of heat transport characteristics due to the dynamics of quantum systems under consideration. Such dynamics is captured by non-steady-state solutions to time-dependent Schrödinger wave equation or by specific solutions of interrelated Pauli rate equations. Since the applicability of Fourier's law is questionable at nanoscale and in the case of transient heat conduction, we pay particular attention to the new physics of post-Fourier heat transport and its further consequences. For instance, the non-equilibrium conditions may establish and maintain certain degree of coherence between correlated quantum states which are involved into the energy conduction process. Understanding and gaining control of coherent manipulations of qubits (two-level quantum systems) is crucial for further development of quantum informatics.

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